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Condensate-profile asymmetry of a boson mixture in a disk-shaped harmonic trap

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A mixture of two types of hard-sphere bosons in a disk-shaped harmonic trap is studied through path-integral quantum Monte Carlo simulation at low temperature. We find that the system can undergo a phase transition to break the spatial symmetry of the model Hamiltonian when some of the model parameters are varied. The nature of such a phase transition is analyzed through the particle distributions and angular correlation functions. Comparisons are made between our calculations and the available mean-field results on similar models. Possible future experiments are suggested to verify our findings.

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Mixtures of different cold atoms are studied intensively by both theorists and experimentalists after the first experimental observation of a stable double condensate formed from two different spin states of ^{87}Rb [1]. Interesting phenomena, such as the formation of molecules, can be directly realized in these mixtures [2, 3]. Furthermore these mixtures form a rich set of systems that can test many-body theory and novel ideas at extremely low temperature and quantum limits [4, 5, 6].

One of the intriguing features predicted to occur in such systems, based on the solutions of the Gross–Pitaevskii equation [7, 8, 9, 10, 11, 12, 13, 14], is the broken spatial symmetry of the Hamiltonian in the condensate profiles of individual species in the system. This is purely a quantum phenomenon because it is not expected in the particle distributions of the corresponding classical systems. It is known that a double condensate can form an inner core from one species and an outer shell from the other in a spherically symmetric trap [15, 16], which is a result of the competition between correlation and coherence presented in the system [17], while preserving the symmetry of the Hamiltonian. But this structure may become unstable for certain interaction strength and total number of particles and the system can undergo a quantum phase transition to a state with a broken spatial symmetry [7, 8]—a double-condensate mixture in an anisotropic trap can develop an asymmetry in condensate profiles along the direction of the weakest confinement, according to the mean-field studies [9, 10, 11, 12, 13, 14]. But it is not entirely certain whether these predications are genuine results of the model system or some artifacts of the mean-field approximation.

In this Letter we report key results from our recent study of the two-component hard-sphere boson mixtures in a disk-shaped harmonic trap through path-integral quantum Monte Carlo simulation, which is exact within a controllable sampling variance. This method allows us to study many-body quantum systems at finite temperature accurately and to make precise predications about the model systems studied. The technique has been applied successfully to boson cluster in various traps [18] and to the two-component system in a harmonic trap that is spherically symmetric [17]. For a double condensate in a disk-shaped harmonic trap, we find that each component can undergo a phase transition and break the spatial symmetry of the Hamiltonian (or that of the trap potential) when certain parameters of the system, such as the interaction range, or the aspect ratio of the axial confinement along the z direction and the radial confinement in the xy plane, are varied. The results are in qualitative agreement with the mean-field studies [9, 10, 11, 12, 13, 14] of this model. In order to understand this symmetry-breaking phenomenon in detail, we analyze the influences of the interaction range, temperature, and number of particles of each species, external potential and elucidate the nature of this phase transition.

Here we consider a two-component mixture of hard-sphere bosons described by the model Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \sum_{j>k=1}^{N} V_{jk}, \tag{1}$$

where

$$\mathcal{H}_i = -\frac{\hbar^2}{2m_i}\sum_{l=1}^{N_i}\nabla_l^2 + \sum_{l=1}^{N_i} U_i(\mathbf{r}_l) \tag{2}$$

is the Hamiltonian of the corresponding noninteracting system under the trapping potential $U_i(\mathbf{r}) = m_i\omega_\perp^2(x^2 + y^2 + \lambda^2 z^2)/2$. The parameter $\lambda = \omega_z/\omega_\perp$ is a measure of the aspect ratio between the axial confinement along the z direction and the radial confinement in the xy plane, with $\omega_\perp = \omega_x = \omega_y$. The system is in the shape of a flat disk if $\lambda \gg 1$ or a long cigar if $\lambda \ll 1$, including the limits $\lambda = 1$ (spherically symmetric), $\lambda = 0$ (confined along the z axis), and $\lambda = \infty$ (confined in the xy plane). The interaction between any two particles V_{jk} is taken to be a hard-sphere potential, modeled after the s-wave scattering lengths of the experimental systems, with a_{11} and a_{22} being the diameters of the particles in species 1 and 2, respectively, and $a_{12} = (a_{11} + a_{22})/2$ being the potential range between two different particles. Masses m_1 and m_2 and total numbers of particles N_1 and N_2 are used for each of the two species, respectively, with

$N = N_1 + N_2$ being the total number of particles in the system.

We performed simulations by carefully choosing the total number of time slices and the size of the Monte Carlo steps to ensure a good convergence of the physical quantities calculated, including the density $\rho_i(\mathbf{r})$ and the in-plane angular pair-correlation function $\Gamma_i(\varphi) = \langle\delta(\varphi - |\varphi_l - \varphi_k|)\rangle$ for $l \neq k$. In order to examine the condensate profiles against the planar symmetry of the trap, we set the temperature much lower than the critical temperature and projected all the particles into the xy plane when we take snapshots or calculate the average radial density $\rho_i(\rho)$ and angular correlation function $\Gamma_i(\varphi)$, where $\rho = \sqrt{x^2 + y^2}$ is the in-plane radius and φ is the relative azimuthal angle. The density is normalized by $2\pi \int_0^\infty \rho_i(\rho)\rho\, d\rho = N_i$.

In Fig. 1 we show three sets of simulation results for different aspect ratio λ under the same trapping frequency for both species at $T/N^{1/3} = 0.1$. It is clear that the symmetry of the Hamiltonian is preserved in the condensate profiles when the trap is spherically symmetric, that is, $\lambda = 1$. For both $\lambda = 4$ and $\lambda = 16$, the profiles are obviously asymmetric with a random orientation due to the spontaneous symmetry-breaking. The asymmetry becomes more severe and the correlation at small angle, as shown in Fig. 1(d), becomes much stronger as the ratio λ increases.

The symmetry-breaking in one species compensates the other because the center of mass of the system, under the given conditions, remains at the center of the trap, resulting in a stronger deformation in the lighter species. We performed one more simulation with $\lambda < 1$ and did not see any symmetry-breaking of the profiles in the xy plane. This is consistent with the findings of previous mean-field calculations [7, 13] based on the Gross–Pitaevskii equation, which concluded that the symmetry is broken in the direction of the weakest trapping frequency.

Let us now examine how the system responses to the change of the ratio $\eta = a_{11}/a_{22}$, which is a measure of the imbalance of the particle sizes between the two species. In Fig. 2 we show three sets of snapshots with different η while having other parameters $m_2/m_1 = 4$, $N_1 = N_2 = 100$, $\lambda = 16$, and $a_{11} = 0.15$ fixed.

For the case of $\eta = 1/3$, the system shows a condensed core of species 1, surrounded by an outer ring of species 2. Both condensates appear to have the planar symmetry of the trap. When η is increased to 1/2, the system undergoes a quantum phase transition from two separate condensates to a binary mixture with each breaking the planar symmetry. This is evident from both snapshots and the correlation functions shown. The correlation at small angle increases when the symmetry is broken. Note that the condensate of species 1 is expected more off-centered (4 times) because the center of mass of the whole system must remain at the trap center. One can

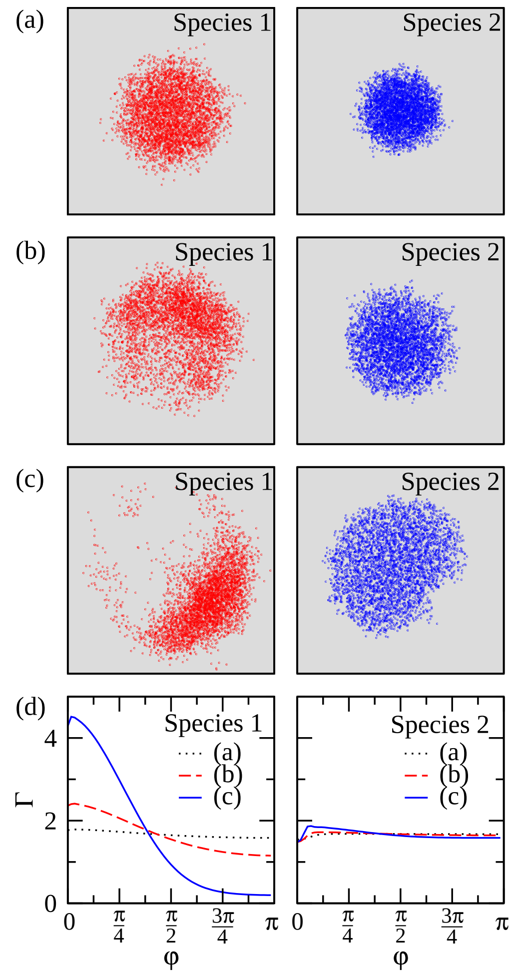

FIG. 1: Snapshots of multi-exposures of the particles viewed along the z direction for each species in a double-condensate mixture, confined in a trap with $m_2/m_1 = 4$, $N_1 = N_2 = 100$, $a_{11} = 0.2$, and $a_{22} = 0.4$, for different aspect ratio $\lambda = \omega_z/\omega_\perp$: (a) $\lambda = 1$; (b) $\lambda = 4$; and (c) $\lambda = 16$. The corresponding in-plane angular pair-correlation functions $\Gamma_i(\varphi)$ are shown in (d). The planar symmetry in each of the two condensates is broken if $\lambda \neq 1$; the asymmetry becomes more severe when λ is further away from 1, especially for the lighter species.

see from the snapshots that the binary phase is formed from the outward movement of species 1 plus the inward movement of species 2. Therefore, increasing η further can result in exchanging the roles of the two species. This is precisely what happens when η is increased to 1—the system shows a condensed core of species 2, surrounded by an outer ring of species 1. The correlation at small angle decreases and the planar symmetry of the Hamiltonian gets restored in the condensate profiles in the same time.

To investigate the temperature dependence of asymmetry of each condensate, we divide the trap into two equal halves by a plane through the z axis, with the low-density side containing a minimum number of particles (N_{L}) and the high-density side containing a maximum

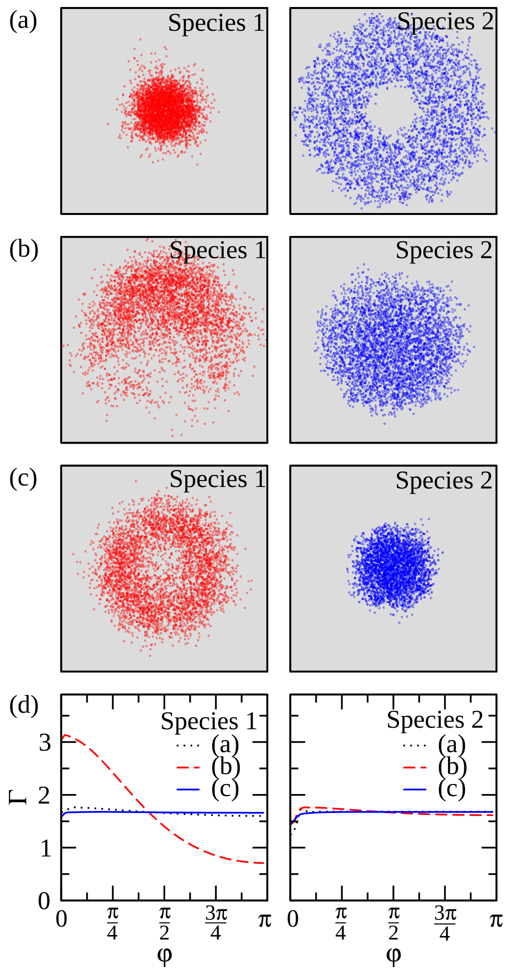

FIG. 2: Snapshots of multi-exposures of the particles viewed along the z direction for each species in a double-condensate mixture, confined in a trap with $m_2/m_1 = 4$, $N_1 = N_2 = 100$, $\lambda = \omega_z/\omega_\perp = 16$, and $a_{11} = 0.15$ fixed, for different ratio $\eta = a_{11}/a_{22}$: (a) $\eta = 1/3$; (b) $\eta = 1/2$; and (c) $\eta = 1$. The corresponding in-plane angular pair-correlation functions $\Gamma_i(\varphi)$ are shown in (d). The planar symmetry of the particle distributions is broken first and then restored when the ratio is varied monotonically.

number of particles ($N_{\rm H}$). Then we examine the ratio $\xi = N_{\rm L}/N_{\rm H}$, which is shown in Fig. 3 for a trap with $\eta = 1/2$, $m_2/m_1 = 4$, $N_1 = N_2 = 100$, and $\lambda = 16$ fixed.

A general feature emerges from all these systems: The asymmetry is depleted in both the extremely low temperature region and high temperature region. The causes are however different. At the extremely low temperature, the strong coherence in each of the condensates forces the particles to go to the lowest single-particle states, and hence to form a nearly symmetric distribution. This is extremely evident from the systems with a weaker interaction, for example, in cases with $a_{11} = 0.1$ and $a_{11} = 0.15$, where the symmetry is nearly completely restored when temperature is lower than $0.05N^{1/3}$. At the high temperature, particles gain more thermal (kinetic)

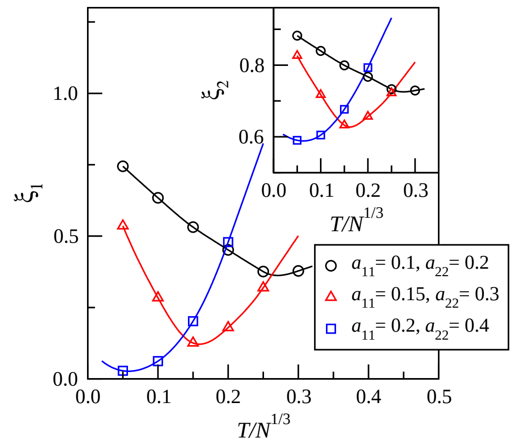

FIG. 3: Temperature dependence of the condensate profile asymmetries, measured from the ratio $\xi = N_{\rm L}/N_{\rm H}$, where $N_{\rm L}$ is the number of the particles in the low-density half and $N_{\rm H}$ is the number of particles in the high-density half, with $\eta = a_{11}/a_{22} = 1/2$, $m_2/m_1 = 4$, $N_1 = N_2 = 100$, and $\lambda = 16$ fixed. The most severe asymmetry for each case happens at a temperature that decreases with the interaction (hard-sphere diameter).

energy and can therefore spread out more in order to distribute more symmetrically. More detailed analysis of the data also show that for weaker interaction cases, the particles from one condensate penetrate into the other condensate when temperature is increased, whereas for the stronger interaction cases, the particles from one condensate go around to form an outer ring.

The optimal temperature, at which the system shows a minimum $N_{\rm L}/N_{\rm H}$ (maximum asymmetry) in Fig. 3, decreases with the interaction range. This is consistent with our earlier findings [17] that the many-body correlation effect, originated from the strong interaction, is in competition with the coherence and it is more difficult to restore the symmetry in the systems with a strong interaction. Another distinctive feature obtained here is that the minimum ratio of $N_{\rm L}/N_{\rm H}$ is smaller if the interaction range is greater. In other words, the system with a stronger interaction can reach a higher asymmetry.

In addition to the interaction and temperature, the structure of a double-condensate mixture also depends on the total number of particles in the system. In Fig. 4, we show the results of three different N_2 while keeping $N_1 = 100$, $m_2/m_1 = 4$, $a_{11} = 0.2$, $a_{22} = 0.4$, and $\lambda = 16$ fixed.

From the correlation functions shown for $N_2 = N_1 = 100$, the particles from species 1 occupy one side of the trap with a significant asymmetry while the particles from species 2 stay at the center of trap with a smaller asymmetry, also seen in Fig. 1 (c). Quantitatively, one expects that the center of mass of species 1 is about four times away from the trap center of that of species 2 in this case because the center of mass of the system is at

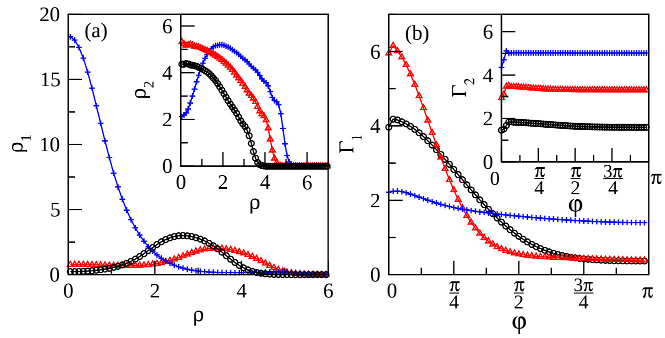

FIG. 4: (a) Density profiles $\rho_i(\rho)$ and (b) angular pair-correlation functions $\Gamma_i(\varphi)$ of the particles confined in a trap with $N_1 = 100$, $m_2/m_1 = 4$, $a_{11} = 0.2$, $a_{22} = 0.4$, and $\lambda = 16$ fixed, for $N_2 = 100$ (circles), 200 (triangles), and 300 (crosses). As N_2 increases, the lighter particles, while maintaining certain asymmetry, contract and are eventually surrounded by the heavier particles that always appear to be distributed symmetrically and are pushed out of the center.

the center of the trap. When N_2 is increased to 200, the particles in species 2 squeeze each other outward but push some of the particles in species 1 into the central area and others further off the center. Finally when N_2 is increased to 300, particles in species 1 all move to the central area; both condensates recover the planar symmetry of the trap with particles in species 2 forming an outer ring, surrounding completely the particles from species 1. However when N_1 is increased from 100 to 300 with N_2 kept to be 100, the asymmetries return with each condensate occupying one side of the trap.

So far we have shown the results with both the species under the same trapping frequency, which means a different external potential for each species if $m_2/m_1 \neq 1$. In order to examine the influence of external potential, we can either choose $m_2/m_1 = 1$ with the same trapping frequency or set $m_1/m_2 = \omega_2^2/\omega_1^2$. Such simulations performed for those systems depicted in Fig. 1 show no broken symmetry as the aspect ratio λ is increased from 1 to 16, although phase separation still occurs along ρ direction. This is similar to the case of our previous work on the double-condensate mixture in a spherically symmetric trap [17]; we also find that the particles with a larger interaction range are in the outer ring while the other condensate stays at the central area.

The external potential plays an important role in the development of asymmetry in the systems studied. For a system with $m_2/m_1 = 4$ under the same trapping frequency, the condensates can undergo a symmetry-to-asymmetry transition and then an asymmetry-to-symmetry transition, as shown in Fig. 2. However, for a system with $m_2/m_1 = 1$, still under the same trapping frequency, no significant asymmetry can be developed. The system with $a_{11}/a_{22} = 0.5$ can have a stable, phase-separated configuration similar to that of Fig. 2(a), which is also a stable configuration obtained in a mean-field approach [8] with $a_{12}/(a_{11}a_{22})^{1/2} \approx 1.06$. Furthermore, when a_{11}/a_{22} is increased to 1, the two separated condensates penetrate each other and form a binary mixture with a slight asymmetry—the double condensates are mirror images of each other because of the interchangeable nature of the two species under the given conditions.

In summary, our simulations show that asymmetry can occur in a double-condensate mixture confined in a disk-shaped trap. The asymmetry has a strong dependence on the aspect ratio of the axial confinement along the z direction and the radial confinement in the xy plane, the ratio of the interaction ranges a_{11}/a_{22}, and the temperature. Furthermore, the total numbers of particles in the two species and significant difference in the external potentials can also affect the structures of the condensates. The novel behavior of a double-condensate mixture elucidated in this work can be verified experimentally with the setup that has created the mixtures and it is extremely interesting to see such phenomena involving quantum phase transition and reentry of symmetry of a model Hamiltonian realized in a laboratory.

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